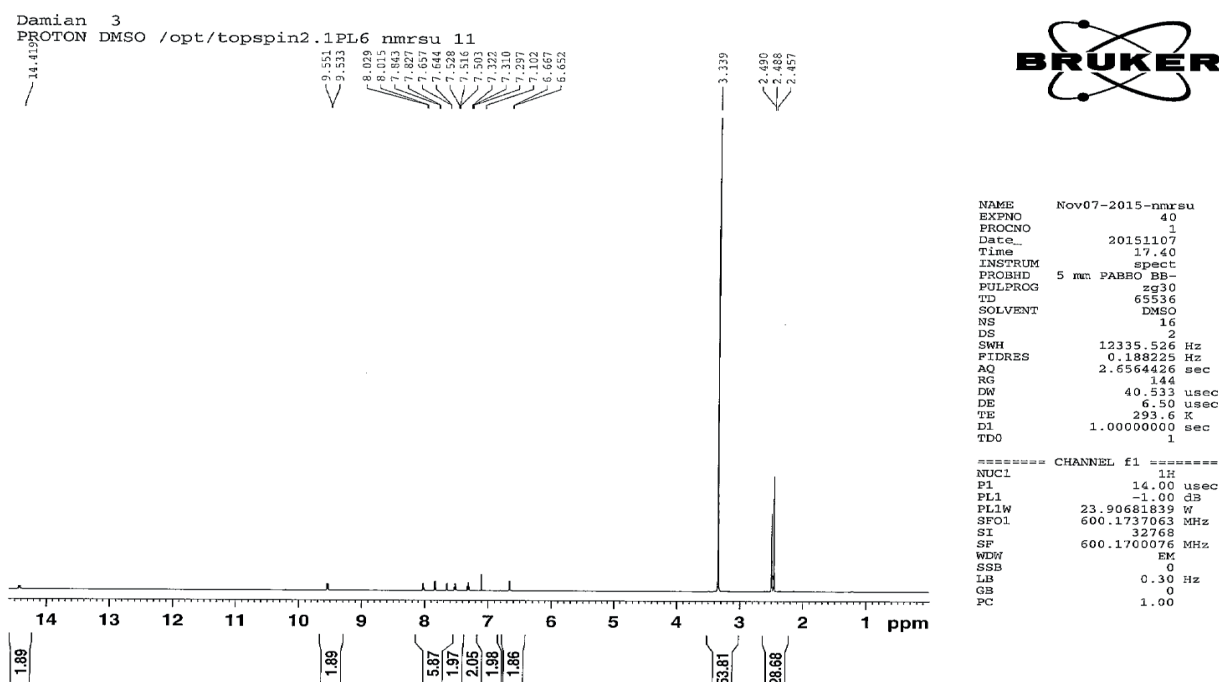


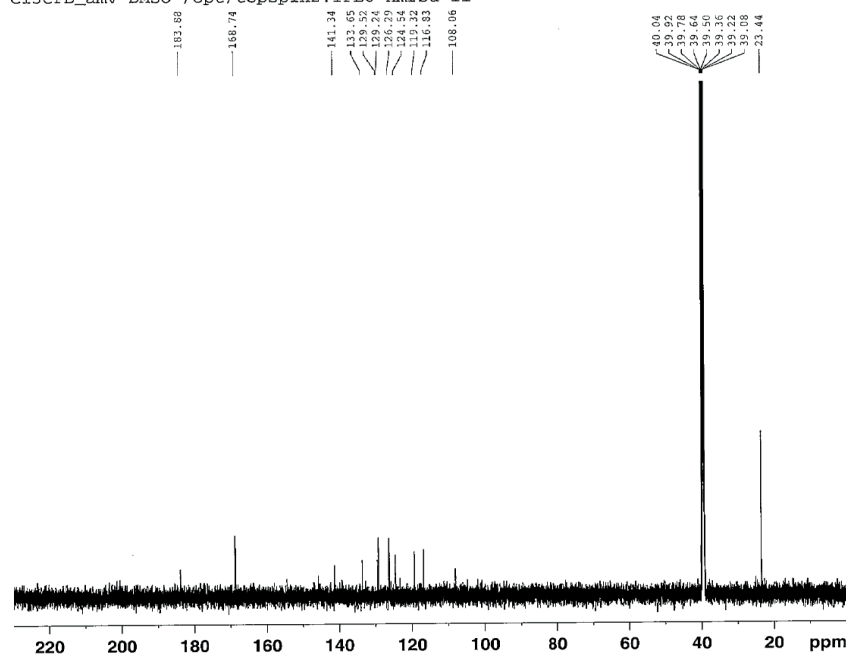
## Supplementary Information

## Open Access

# Supplement: Synthesis, characterization, *in-vitro* antimicrobial properties, molecular docking and DFT studies of 3-{(E)-[(4,6-dimethylpyrimidin-2-yl)imino]methyl}naphthalen-2-ol and Heteroleptic Mn(II), Co(II), Ni(II) and Zn(II) complexes



Damian 3  
C13CPD\_amv DMSO /opt/topspin2.1PL6 nmrsu 11



```

NAME      Nov07-2015-nmrsu
EXPNO     41
PROCNO    1
Date_     20151107
Time      17.54
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        36057.691 Hz
FIDRES     0.550197 Hz
AQ         0.9088159 sec
RG         2050
DW         13.867 usec
DE         6.50 usec
TE         294.5 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         10.00 usec
PL1        -1.00 dB
PL1W       48.09095001 W
SFO1       150.9300706 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      95.00 usec
PL2        -1.00 dB
PL12       16.08 dB
PL13       19.00 dB
PL2W       23.80681839 W
PL12W      0.46829745 W
PL13W      0.23906820 W
SFO2       600.1724007 MHz
SI         32768
SF         150.9129354 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```



## Mass Spectrum SmartFormula Report



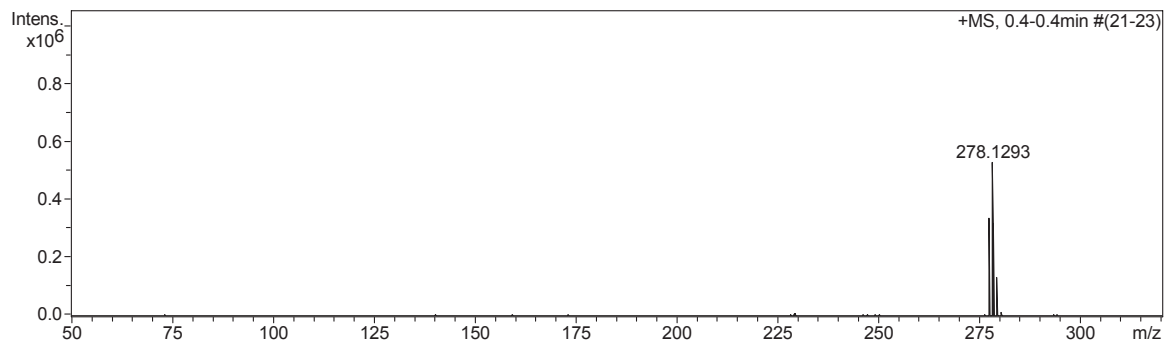
### Analysis Info

Analysis Name D:\Data\06112015\LADMS000003.d  
Method tune\_low20102015.m  
Sample Name HL3  
Comment

Acquisition Date 11/6/2015 10:32:21 AM  
Laboratory Laboratory for Analytical Services  
Operator JHL Jordaan  
Instrument / Ser# micrOTOF-Q II 10390

### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	N-Rule	e <sup>-</sup> Conf
278.1293	1	C 17 H 16 N 3 O	100.00	278.1288	-0.5	-1.9	31.7	11.5	ok	even